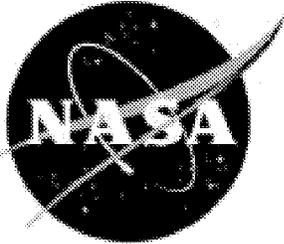


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Equivalent-Continuum Modeling With Application to Carbon Nanotubes

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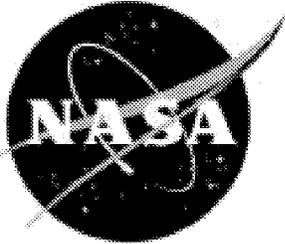
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Equivalent-Continuum Modeling with Application to Carbon Nanotubes

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Abstract

A method has been proposed for developing structure-property relationships of nano-structured materials. This method serves as a link between computational chemistry and solid mechanics by substituting discrete molecular structures with equivalent-continuum models. It has been shown that this substitution may be accomplished by equating the molecular potential energy of a nano-structured material with the strain energy of representative truss and continuum models. As important examples with direct application to the development and characterization of single-walled carbon nanotubes and the design of nanotube-based structural devices, the modeling technique has been applied to two independent examples: the determination of the effective-continuum geometry and bending rigidity of a graphene sheet. A representative volume element of the chemical structure of graphene has been substituted with equivalent-truss and equivalent-continuum models. As a result, an effective thickness of the continuum model has been determined. The determined effective thickness is significantly larger than the inter-planar spacing of graphite. The effective bending rigidity of the equivalent-continuum model of a graphene sheet was determined by equating the molecular potential energy of the molecular model of a graphene sheet subjected to cylindrical bending (to form a nanotube) with the strain energy of an equivalent-continuum plate subjected to cylindrical bending.

KEY WORDS: nanotechnology, nanotubes, continuum mechanics, molecular mechanics, flexural rigidity, graphene sheet

Nomenclature

Molecular model and force field

- E^{el} - Non-bonded electrostatic potential energy
- E^g - Molecular potential energy of graphene sheet
- E^{nsm} - Potential energy of nano-structured material
- E^{vdW} - Non-bonded van der Waals potential energy
- E^θ - Bond-angle variation potential energy
- E^p - Bond stretching potential energy
- E^τ - Bond torsion potential energy
- E^ω - Bond inversion potential energy
- K_m^p - Force constant associated with the stretching of bond m
- K_m^θ - Force constant associated with angle variation of bond angle m

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- K^{ω} - Force constant associated with bond inversion
 $\overline{K^{\omega}}$ - Modified force constant associated with bond inversion
 L - Length of carbon nanotube
 N - Number of atoms per carbon nanotube
 p - Total number of carbon atoms in carbon structure
 α - Interatomic spacing of carbon atoms in graphite
 r^{nt} - Radius of carbon nanotube
 $\overline{\Phi_p}$ - Average inversion angle (radians)
 $\Phi_{\sigma\pi}$ - Angle between σ and π bonds
 θ_m - Deformed bond-angle m
 Θ_m - Equilibrium bond-angle m
 ρ_m - Deformed bond length of bond m
 P_m - Equilibrium bond length of bond m

Truss and continuum models

- a - Elastic rod type of outer portion of truss representative volume element
 A_m^n - Cross-sectional area of rod m of truss member type n
 A^{nt} - Cross-sectional area of carbon nanotube
 b - Elastic rod type of inner portion of truss representative volume element
 D - Bending rigidity of a continuum plate
 I - Moment of inertia of a continuum plate
 r_m^n - Deformed distance between joints of rod m of truss member type n
 R_m^n - Undeformed distance between joints of rod m of truss member type n
 t - Thickness of a continuum plate (wall thickness of continuum tube)
 Y^g - Young's modulus of graphene sheet
 Y_m^n - Young's modulus of rod m of truss member type n
 Y^{nt} - Young's modulus of carbon nanotube
 r^c - Mid-plane radius of continuum nanotube wall
 r_i^c - Inner radius of continuum nanotube wall
 r_o^c - Outer radius of continuum nanotube wall
 Λ^c - Mechanical strain energy of the continuum model
 Λ^t - Mechanical strain energy of the truss model
 ν - Poisson's ratio of graphene sheet

Boundary conditions

- u_i - Displacement components of equivalent-continuum representative volume element
 x_i - Cartesian coordinate system of the representative volume element

- ε_{ij} - Strain components in the equivalent-continuum representative volume element
- ε - Applied strain
- γ - Applied shear strain

1. Introduction

Nano-structured materials have generated considerable interest in the materials research community in the last few years partly due to their potentially remarkable mechanical properties [1]. In particular, materials such as carbon nanotubes, nanotube and nanoparticle-reinforced polymers and metals, and nano-layered materials have shown considerable promise. For example, carbon nanotubes could potentially have a Young's modulus as high as 1 TPa and a tensile strength approaching 100 GPa. The design and fabrication of these materials are performed on the nanometer scale with the ultimate goal to obtain highly desirable macroscopic properties.

One of the fundamental issues that needs to be addressed in modeling macroscopic mechanical behavior of nano-structured materials based on molecular structure is the large difference in length scales. On the opposite ends of the length scale spectrum are computational chemistry and solid mechanics, each of which consists of highly developed and reliable modeling methods. Computational chemistry models predict molecular properties based on known quantum interactions, and computational solid mechanics models predict the macroscopic mechanical behavior of materials idealized as continuous media based on known bulk material properties. However, a corresponding model does not exist in the intermediate length scale range. If a hierarchical approach is used to model the macroscopic behavior of nano-structured materials, then a methodology must be developed to link the molecular structure and macroscopic properties. Even though there is a long history of modeling bulk properties of materials based on molecular properties, a simple link between the firmly established disciplines of computational chemistry and solid mechanics has not been established.

In this paper, a methodology for linking computational chemistry and solid mechanics models has been developed. This tool allows molecular properties of nano-structured materials obtained through molecular mechanics models to be used directly in determining the corresponding bulk properties of the material at the macroscopic scale. The advantages of the proposed method are its simplicity and direct connection with computational chemistry and solid mechanics.

In addition, the proposed method has been demonstrated with two independent examples that have direct application to the development and characterization of single-walled carbon nanotubes (SWNT). First, the effective geometry of a graphene sheet has been determined. A representative volume element (RVE) of the graphene layer has been modeled as a continuous plate with an effective thickness that has been determined from the bulk in-plane properties of graphite [2]. Second, the effective bending rigidity of a graphene sheet has been determined. The bending rigidity of the elastic plate has been described in terms of the atomic interactions that dominate the overall bending behavior.

2. Carbon nanotubes

In 1991 Iijima [3] obtained transmission electron micrographs of elongated, nano-sized carbon particles that consisted of cylindrical graphitic layers, known today as carbon nanotubes (Figure 1). Since then, carbon nanotubes have become a primary focus in nanotechnology research due to their apparent exceptionally high stiffness and strength [1]. One of the fundamental issues that scientists and engineers are confronting is the characterization of the mechanical behavior of individual carbon nanotubes. Two independent components of this issue, the wall thickness and bending rigidity of carbon nanotubes, are discussed below.

2.1 Wall thickness

Many experimental [4-8] and theoretical [9-13] studies have been performed on single- and multi-walled carbon nanotubes. In particular, deformation modes and nanotube stiffnesses have been closely examined.

Physical properties, such as effective cross-sectional area and moment of inertia, and mechanical properties, such as Young's modulus and Poisson's ratio, are traditionally associated with the macroscopic-length scale, where the characteristic dimensions of a continuum solid are well defined. The determination of these properties has been attempted in many of the studies cited above without proper regard to an acceptable definition of the nanotube geometry. Accurate values of macroscopic physical and mechanical properties are crucial in establishing a meaningful link between nanotube properties and the properties of larger structures, such as nanotube-reinforced polymer composites. Therefore, caution should be used when applying continuum-type properties to nano-structured materials.

In many studies, it has been assumed that the nanotube "wall thickness" is merely the inter-planar spacing of two or more graphene sheets [5, 8-13], which is about 0.34 nm in single-crystal graphite. While this simple idealization appears to have intuitive merit, it does not necessarily reflect the *effective* thickness that is representative of continuum properties. In order to avoid this problem, Hernandez *et al.* [10] proposed the use of a specific Young's modulus, i.e., Young's modulus per unit thickness. Even though this approach is convenient for studies concerned with the relative stiffnesses of nanotubes, it is of little use when modeling a nanotube as a continuum structure. Another proposed solution to this dilemma is to assume that the nanotube is a solid cylinder [14-16]. This method is certainly convenient, however, significant inconsistencies arise when comparing moduli data of single wall nanotubes (SWNT) and multi-walled nanotubes (MWNT) when both are assumed to be solid cylinders.

It follows that in order to properly model the mechanical behavior of a SWNT using continuum mechanics, the effective geometry must be known. If the nanotube is modeled as a continuous hollow cylinder with an effective wall thickness, then a simple first step is to model the flat graphene sheet in order to determine the effective wall thickness. In the current study, the effective thickness will be calculated as an example of the proposed modeling approach.

2.2 Bending rigidity

Due to the aspect ratio and tube-like geometry of SWNT, many studies have been conducted concerning the buckling and bending response of nanotubes using both theoretical [12, 14, 16-19] and experimental [20, 21] approaches. In particular, Overney et al. [17] conducted a computational study and calculated a bending parameter of a graphene sheet based on the vibrational modes of a nanotube. Yakobson et al. [18] used computational methods to study the buckling of carbon nanotubes. They modeled the nanotubes as shells with a bending rigidity proportional to the Young's modulus and shell-wall thickness. Using the computationally obtained bending parameters, they calculated the Young's modulus and wall thickness of the shell. Govindjee and Sackman [16] theoretically investigated the validity of continuum mechanics at the nano-scale by examining the bending of multi-walled carbon nanotubes. They also assumed that the bending rigidity of each layer is proportional to the Young's modulus and moment of inertia. In each of these studies it is clear that the bending and buckling behavior of carbon nanotubes is highly dependent on the bending properties of the graphene sheet. Therefore, it follows that the bending behavior of a graphene sheet must be well-understood, and should be described in terms of the atomic properties of graphene.

According to the classical elasticity theory, it is assumed that the bending rigidity, D , of an isotropic solid is related to the cross-sectional geometry and the in-plane modulus [22]:

$$D = \frac{Y^g t^3}{12(1-\nu^2)} \quad (1)$$

and

$$D = Y^g I \quad (2)$$

which are for the bending of plates and beams, respectively. In equations (1) and (2), Y^g , ν , I , and t are the Young's modulus, Poisson's ratio, moment of inertia, and plate thickness of a graphene sheet, respectively. It seems logical that these equations could describe the bending properties of graphene sheets and nanotubes due to geometric similarities to solid plates and/or beams. However, Ru [19] has pointed out that a discrepancy exists in the use of equation (1) when describing bending properties of carbon nanotubes. If the bending rigidity described by this equation is used in the bending analysis of carbon nanotubes, then an equivalent wall thickness must be used that is very small compared to the inter-planar spacing of graphene sheets. For example, Yakobson *et al.* [18] performed molecular dynamics simulations and showed that the bending rigidity of carbon nanotubes is much smaller than that described by equation (1) if the typically assumed effective thickness of 0.34 nm (the inter-plane spacing of layers of graphite) of graphene sheets is used. They derived an effective thickness of 0.066 nm based on an assumed value for Young's modulus of the nanotube (5.5 TPa). The argument of Ru [19] is further supported by examining the chemical structure of a graphene sheet. At first glance, it appears that a graphene sheet would have very little bending rigidity since the atomic C-C bonds lie very close to the neutral axis during cylindrical bending, unlike continuous elastic plates in which there is material that is not on the neutral axis that contributes a resistance in bending that is proportional to the in-plane Young's modulus (equations (1) and (2)). Therefore,

the primary atomic bonds, which are the main contribution to the in-plane elastic properties of graphene, should provide little, perhaps negligible, contribution to the bending rigidity of graphene sheets. The resistance to bending must be due to a different atomic interaction, which is discussed in section 5.

3. Modeling procedure

The proposed method of modeling nano-structured materials with an equivalent-continuum is outlined below. Since the approach uses the energy terms that are associated with molecular mechanics modeling, a brief description of molecular mechanics is given first followed by an outline of the equivalent-truss and equivalent-continuum model development.

3.1 Molecular mechanics

An important component in molecular mechanics calculations of the nano-structure of a material is the description of the forces between individual atoms. This description is characterized by a force field. In the most general form, the total molecular potential energy, E^{nsm} , for a nano-structured material is described by the sum of many individual energy contributions:

$$E^{nsm} = E^p + E^\theta + E^\tau + E^\omega + E^{vdW} + E^{el} \quad (3)$$

where E^p , E^θ , E^τ , and E^ω are the energies associated with bond stretching, angle variation, torsion, and inversion, respectively (the reader should refer to a molecular mechanics text, e.g. [23], for a detailed description of these energy terms). The nonbonded interaction energies consist of van der Waals, E^{vdW} , and electrostatic, E^{el} , terms. Various functional forms may be used for these energy terms depending on the particular material and loading conditions considered [23]. Obtaining accurate parameters for a force field amounts to fitting a set of experimental or calculated data to the assumed functional form, specifically, the force constants and equilibrium structure. In situations where experimental data are either unavailable or very difficult to measure, quantum mechanical calculations can be a source of information for defining the force field.

3.2 Truss model

In order to simplify the calculation of the total molecular potential energy of molecular models with complex molecular structures and loading conditions, an intermediate model may be used to substitute for the molecular model. Due to the nature of molecular force fields, a pin-jointed truss model may be used to represent the energies given by equation (3), where each truss member represents the forces between two atoms. Therefore, a truss model allows the mechanical behavior of the nano-structured system to be accurately modeled in terms of displacements of the atoms. This mechanical representation of the lattice behavior serves as an intermediate step in linking the molecular potential with an equivalent-continuum model. In the truss model, each truss element corresponds to a chemical bond or a significant non-bonded interaction. The stretching potential of each bond corresponds with the stretching of the corresponding truss element. Traditionally, atoms in a lattice have been viewed as masses that are held in place with atomic forces that resemble elastic springs [24]. Therefore, bending of

truss elements is not needed to simulate the chemical bonds, and it is assumed that each truss joint is pinned, not fixed.

The mechanical strain energy, Λ^t , of the truss model is expressed in the form:

$$\Lambda^t = \sum_n \sum_m \frac{A_m^n Y_m^n}{2R_m^n} (r_m^n - R_m^n)^2 \quad (4)$$

where A_m^n and Y_m^n are the cross-sectional area and Young's modulus, respectively, of rod m of truss member type n . The term $(r_m^n - R_m^n)$ is the stretching of rod m of truss member type n , where R_m^n and r_m^n are the undeformed and deformed lengths of the truss elements, respectively.

In order to represent the chemical behavior with the truss model, equation (4) must be equated with equation (3) in a physically meaningful manner. Each of the two equations are sums of energies for particular degrees of freedom. The main difficulty in the substitution is specifying equation (4), which has stretching terms only, for equation (3), which also has bond-angle variance and torsion terms. No generalization can be made for overcoming this difficulty for every nano-structured system. A feasible solution must be determined for a specific nano-structured material depending on the geometry, loading conditions, and degree of accuracy sought in the model.

3.3 Equivalent-continuum model

For many years, researchers have developed methods of modeling large-area truss structures with equivalent-continuum models [25-30]. These studies indicate that various methods and assumptions have been employed in which equivalent-continuum models have been developed that adequately represent truss structures. In general, the equivalent-continuum model is defined as a continuum that has the following characteristics:

1. Truss lattices with pinned joints are modeled as classical continua where micropolar [31] continuum assumptions are not necessary.
2. Local deformations are accounted for.
3. The temperature distribution, loading and boundary conditions of the continuum model simulate those of the truss model.
4. The same amount of thermoelastic strain energy is stored in the two models when deformed by identical static loading conditions.

The parameters of the equivalent-continuum model, such as the elastic properties and geometry, are determined based on the above characteristics. In some cases the strain energy of the continuum, Λ^c , can be easily formulated analytically and compared directly with equation (4) to obtain the equivalent-continuum properties. In other cases, especially with complex geometries and deformations, numerical tools need to be used to determine the continuum parameters. Once the properties of the equivalent-continuum model have been determined, the mechanical

behavior of larger structures consisting of the nano-structured material may be predicted using the standard tools of continuum mechanics.

4. Example 1: Effective geometry of a graphene sheet

In this section, a graphene sheet is modeled as a continuous plate with a finite thickness that represents the effective thickness for the determination of continuum-type mechanical and physical properties. By using the methodology described above, the molecular mechanics model is substituted with a truss model and subsequently an equivalent-plate model. The continuum model may then be used in further solid mechanics-based analyses of SWNT.

4.1 Representative volume element

To reduce the computational time associated with modeling the graphene sheet, a representative volume element (RVE) for graphene was used in this study (Figure 2). The selected RVE allows each degree of freedom of the carbon atom associated with bond stretching and bond-angle variation in the hexagonal ring to be completely modeled by truss and continuum finite element model nodal-displacement degrees of freedom. Also, this RVE allows the displacements on the boundary of the proposed chemical, truss, and continuum models to correspond exactly. Furthermore, macroscopic loading conditions applied to a continuous graphene plate can be easily reduced to periodic boundary conditions that are applied to the RVE.

4.2 Molecular mechanics model

The specific forms of the energy terms in equation (3) used in this example were taken from the AMBER force field of Kollman and coworkers [32, 33]. Due to the nature of the material and loading conditions in the present study, only the bond stretching and bond-angle variation energies were included. Torsion, inversion, and non-bonded interactions were assumed to be negligible for the case of a graphene lattice subjected to small deformations. For this example, the molecular potential energy of a graphene sheet with carbon-to-carbon bonds is expressed as a sum of simple harmonic functions:

$$E^g = \sum_m K_m^\rho (\rho_m - P_m)^2 + \sum_m K_m^\theta (\theta_m - \Theta_m)^2 \quad (5)$$

where the terms P_m and Θ_m refer to the undeformed interatomic distance of bond m and the undeformed bond-angle m , respectively. The quantities ρ_m and θ_m are the bond length and bond-angle after stretching, respectively (see Figure 3). K_m^ρ and K_m^θ are the force constants associated with the stretching and angle variance of bond and bond-angle m , respectively. Using the parameters for the AMBER force field [32], the force constants used in this example are:

$$\begin{aligned}
K^{\rho} &= 46900 \frac{\text{kcal}}{\text{mole} \cdot \text{nm}^2} = 3.26 \cdot 10^{-7} \frac{\text{nJ}}{\text{bond} \cdot \text{nm}^2} \\
K^{\theta} &= 63 \frac{\text{kcal}}{\text{mole} \cdot \text{rad}^2} = 4.38 \cdot 10^{-10} \frac{\text{nJ}}{\text{angle} \cdot \text{rad}^2}
\end{aligned} \tag{6}$$

The equilibrium bond length, P_m , is 0.140 nm, and the undeformed bond-angle, Θ_m , is 120.0 degrees.

4.3 Truss model

In order to express the mechanical strain energy, Λ^t , of the truss model in terms of the variable truss joint angles that are specified in molecular mechanics ($\theta_m - \Theta_m$), the RVE has been modeled with additional rods between nearly adjacent joints to represent the interaction between the corresponding carbon atoms (Figure 3). In order to represent the chemical model, which has bond stretching and variable angles as degrees of freedom, with a truss model that has stretching degrees of freedom only, two types of elastic rods, a and b , are incorporated into the truss RVE.

The mechanical strain energy, Λ^t , of the discrete truss system shown in Figure 3 is expressed in the form of equation (4) as:

$$\Lambda^t = \sum_m \frac{A_m^a Y_m^a}{2R_m^a} (r_m^a - R_m^a)^2 + \sum_m \frac{A_m^b Y_m^b}{2R_m^b} (r_m^b - R_m^b)^2 \tag{7}$$

where the superscripts correspond to rod types a and b , respectively. Comparing equations (5) and (7), it is clear that the bond stretching term in the equation (5) can be related to the first term of equation (7) for the rods of type a :

$$K_m^{\rho} = \frac{A_m^a Y_m^a}{2R_m^a} \tag{8}$$

where it is assumed that $\rho_m = r_m^a$ and $P_m = R_m^a$. However, the second terms in equations (5) and (7) cannot be related directly. In order to equate the constants, the chemical bond-angle variation must be expressed in terms of the elastic stretching of the truss elements of type b . For simplicity, it may be assumed that the prescribed loading conditions consist of small, elastic deformations only. This assumption is not an over-simplification for the graphene sheet since the deformations for highly stiff linear-elastic materials subjected to many practical loading conditions are quite small.

In order to express the Young's modulus of the rods of type b in terms of the bond-angle force constant, a relationship between the change in the bond angle and the corresponding change in length of the type b truss element is required. If it is assumed that the changes in bond angle are small, then it can be easily shown that (see Figure 4):

$$\theta_m - \Theta_m \approx \frac{2(r_m^b - R_m^b)}{R_m^a} \quad (9)$$

The right-hand side of equation (9) is four times larger than the right hand side of equation (8) given by Odegard *et al.* [34]. This discrepancy is due to an improvement in the assumptions used to derive equation (9) in the current study. Substitution of equation (9) into equations (5) and (7) results in the following approximation:

$$K_m^\theta = \frac{R_m^b A_m^b Y_m^b}{24} \quad (10)$$

Therefore, the Young's moduli of the two rod types are:

$$\begin{aligned} Y_m^a &= \frac{2K_m^p R_m^a}{A_m^a} \\ Y_m^b &= \frac{24K_m^\theta}{R_m^b A_m^b} \end{aligned} \quad (11)$$

The strain energy of the truss model may then be expressed in terms of the force constants:

$$\Lambda^t = \sum_m K^p (r_m^a - R_m^a)^2 + \sum_m \frac{12K^\theta}{(R_m^b)^2} (r_m^b - R_m^b)^2 \quad (12)$$

4.4 Equivalent-plate model

Working with the assumptions discussed herein, the next step in linking the molecular and continuum models is to replace the equivalent-truss model with an equivalent-continuous plate with a finite thickness (Figure 3). For this example, it is assumed that the truss and continuum models are equivalent when the elastic strain energy stored in the two models are equal under identical displacement boundary conditions. The value of the plate thickness that results in equal strain energies is the assumed effective thickness of the graphene sheet.

While the mechanical properties of the truss elements have been determined as described above, those of the graphene sheet were taken from the literature. Values for the in-plane mechanical properties of graphite have been measured macroscopically, i.e., without any assumptions regarding the graphene sheet thickness. For this example, the values of the mechanical properties are [2]:

$$\begin{aligned} Y^g &= 1008 \text{ GPa} \\ \nu &= 0.145 \end{aligned} \quad (13)$$

where Y^g and ν are the Young's modulus and Poisson's ratio of graphite, respectively. For simplicity, it is assumed that graphite is isotropic since no out-of-plane deformations are considered here. The isotropic properties of the graphene sheet in equation (13) are based on the in-plane properties of bulk graphite.

4.5 Boundary conditions

In order to determine an effective plate thickness, both the truss and continuum models were subjected to three sets of loading conditions. For each set of loading conditions, a corresponding effective thickness was determined. The loading conditions correspond to the three fundamental in-plane deformations of a plate, that is, uniform axial tension along x_1 and x_2 and pure shear loading in the x_1 and x_2 plane.

For a uniaxial deformation along the x_2 direction (load case I), the RVE may be subjected to the following boundary conditions (Figure 5):

$$\begin{aligned} u_1 &= -\nu \epsilon x_1 \\ u_2 &= \epsilon x_2 \\ u_3 &= -\nu \epsilon x_3 \end{aligned} \quad (14)$$

where the displacement components are parallel to the corresponding RVE coordinates. The total strain energy can be calculated using [22]:

$$\Lambda^c = \frac{VY^g}{2(1+\nu)} \left[\frac{\nu}{1-2\nu} \epsilon_{kk}^2 + \epsilon_{ij} \epsilon_{ij} \right] \quad (15)$$

where V is the volume of the RVE, $i, j, k = 1, 2, 3$ (using summation notation), and the components of the strain tensor, ϵ_{ij} , are given by:

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \quad (16)$$

For the RVE under the conditions given in equation (14):

$$\Lambda^c = \frac{3\sqrt{3}}{4} (R^a)^2 t Y^g \epsilon^2 \quad (17)$$

where t is the thickness of the continuum plate. For a uniaxial deformation along the x_1 direction (load case II), the boundary conditions are (Figure 6):

$$\begin{aligned}
u_1 &= \varepsilon x_1 \\
u_2 &= -\nu \varepsilon x_2 \\
u_3 &= -\nu \varepsilon x_3
\end{aligned} \tag{18}$$

The total strain energy of an equivalent-continuum RVE under this condition is given by equation (17). For a pure shear strain in the x_1 - x_2 plane (Load case III), the RVE may be subjected to the following boundary conditions (Figure 7):

$$\begin{aligned}
u_1 &= 0 \\
u_2 &= \gamma x_1 \\
u_3 &= 0
\end{aligned} \tag{19}$$

The total strain energy of an equivalent-continuum RVE under this condition is:

$$\Lambda^c = \frac{3\sqrt{3}}{8} (R^a)^2 t \frac{Y^g}{(1+\nu)} \gamma^2 \tag{20}$$

4.6 Results and discussion

The strain energy of the truss model was calculated using a finite element analysis (ANSYS 5.7[®] [35]) for all three boundary conditions. The strain energies of each truss element were summed to obtain the total strain energy for the RVE. The resulting strain energy was equated with equations (17) or (20) for Load cases I and II or III, respectively, and the corresponding effective thickness of the equivalent-continuum plate, t , was determined. Each extensible rod was modeled using a finite truss element (LINK1) with two degrees of freedom at each node (displacements parallel to x_1 and x_2). The cross-sectional areas of the type a rods were divided by a factor of 2, since these rods are sharing their total area with adjacent RVEs. For Load cases I and II, the resulting effective thickness was calculated to be 0.69 nm. For Load case III, the effective thickness was 0.57 nm. These values are significantly larger than the widely accepted value for the graphitic inter-planar spacing, 0.34 nm, and much larger than the value suggested by Yakobson *et al.* [18], 0.066 nm.

It may be assumed that during uniaxial loading of a carbon nanotube, with the force and strain known, the Young's modulus can be calculated using:

$$Y^{nt} \propto (A^{nt})^{-1} \tag{21}$$

where A^{nt} is the cross-sectional area of the hollow continuum cylinder with a constant mid-plane radius, r^c . The inner radius, r_i^c , and outer radius, r_o^c , of the tube are (Figure 8):

$$\begin{aligned} r_i^c &= r^c - \frac{t}{2} \\ r_o^c &= r^c + \frac{t}{2} \end{aligned} \quad (22)$$

where $r^c \geq t/2$. The cross-sectional area of the hollow continuum cylinder is:

$$A^{nt} = 2\pi r^c t \quad (23)$$

The calculated cross-sectional areas using the effective thickness values obtained above are shown in Table 1. The ratios of the calculated Young's modulus based on the effective thickness obtained for the three load cases, their average, and from Yakobson *et al.* [18], to the Young's modulus based on inter-planar spacing, are also provided in Table 1. The results shown in Table 1 suggest that measured and calculated values of mechanical properties of carbon nanotubes that are dependent on the dimensions of the continuum tube may differ significantly based on the assumed geometry.

5. Example 2: Effective bending rigidity of a graphene sheet

In this section, a graphene sheet is again modeled as a continuous plate. The bending rigidity of the plate is assumed to be independent of the in-plane mechanical properties and thickness of the plate. By using the proposed modeling method, the molecular mechanics model is used to determine the effective bending rigidity of the continuum plate.

5.1 Molecular mechanics model

It has been shown that the only significant change in the electronic structure of a flat graphene sheet when subjected to pure bending is the change in the π -orbital electron density on either side of the graphene sheet (i.e. inversion, see Figure 9) [36-41]. This indicates that the inversion alone contributes to the bending resistance of graphene sheets. Bakowies and Theil [36] have suggested that the increase in the total molecular potential energy per carbon atom of a carbon cluster (i.e. a structure formed by a single plane of carbon atoms, such as carbon Fullerenes and SWNT) with respect to a flat graphene sheet may be closely approximated as:

$$E^{\omega} = K^{\omega} \bar{\phi}_p^2 \quad (24)$$

where K^{ω} is a force constant and $\bar{\phi}_p$ is the average inversion angle defined as (in radians):

$$\bar{\phi}_p = \frac{\sum_p \left(\phi_{\sigma\pi} - \frac{\pi}{2} \right)}{p} \quad (25)$$

where p is the total number of carbon atoms in the carbon structure considered and $\phi_{\sigma\pi}$ is the angle defined in Figure 9. For simplicity in the specific case of carbon nanotubes, the π -orbital

axis vector technique [42] can be used to show that the change in the molecular potential energy due to inversion can be expressed in terms of the nanotube radius, r^{nt} :

$$E^{\omega} = \frac{\overline{K^{\omega}}}{(r^{nt})^2} \quad (26)$$

where $\overline{K^{\omega}}$ is a modified inversion force constant given by:

$$\overline{K^{\omega}} = (0.0012 \text{ rad}^2 \text{ nm}^2) K^{\omega} \quad (27)$$

Values of the force constant, $\overline{K^{\omega}}$, have been determined using computational chemistry data from several studies [36, 43-46] and equation (26). The values are shown in Table 2 along with the overall average, which is:

$$\overline{K^{\omega}} = 0.018 \frac{eV \cdot \text{nm}^2}{\text{atom}} \quad (28)$$

The total number of carbon atoms per nanotube is [43]:

$$N = \frac{4\pi r^{nt} L^{nt}}{3\alpha^2} \quad (29)$$

where α is the interatomic spacing of carbon atoms and L^{nt} is the nanotube length. Therefore, the total change in the molecular potential energy of a nanotube due to inversion is:

$$E^{\omega} N = \frac{4\pi L^{nt} \overline{K^{\omega}}}{3\alpha^2 r^{nt}} \quad (30)$$

5.2 Equivalent-continuum plate

In the case of a graphene sheet subjected to pure bending, the total molecular potential energy is easily described with a single force constant by using equation (30), unlike the example discussed in the previous section where an intermediate truss model was needed in order to calculate the strain energy under various loading conditions. Therefore, the truss model is not needed in this particular example and an equivalent-continuum model has been developed by equating the total molecular potential energy of the molecular model and the strain energy of the continuum plate directly.

The strain energy of a plate of length L^c subjected to cylindrical curvature (Figure 8) is [47]:

$$\Lambda^c = \frac{\pi D L^c}{r^c} \quad (31)$$

where r^c is the radius of curvature, D is the bending rigidity, and the superscript c denotes the strain energy associated with the continuum plate. In this case, D is not defined by equations (1) or (2) for the reasons discussed above. In order to determine the bending rigidity of the equivalent-continuum plate that represents the actual effective bending rigidity of the graphene sheet, the strain energy of the continuum plate and the increase in the total molecular potential energy of the graphene sheet must be equivalent when subjected to pure bending. Equating equations (30) and (31) results in:

$$D = \frac{4\overline{K^\omega}}{3\alpha^2} \quad (32)$$

Therefore, the effective bending rigidity is directly proportional to the inversion force constant and the inverse square of the interatomic spacing of graphite.

The equivalent bending rigidity for the equivalent-continuum plate is calculated using equation (32) and the average value of the force constant $\overline{K^\omega}$, given in Table 2, and with $\alpha = 0.140$ nm [2] to give $D = 1.22$ eV. This value is 44% higher than that used by Yakobson *et al.* [18] and Robertson *et al.* [43] ($D = 0.85$ eV).

The strain energy of a graphene sheet is presented in Figure 10 for different nanotube radii for all of the computational chemistry data and the equivalent continuum plate model. It is assumed that the graphene sheet behaves elastically in bending for all nanotube radii. Clearly, the trends of the computational chemistry data and the equivalent-continuum model are in agreement.

6. Summary

A method has been presented for modeling structure-property relationships of nano-structured materials. This method serves to link computational chemistry, which is used to predict molecular properties, and solid mechanics, which describes macroscopic mechanical behavior based on bulk material properties. This link is established by replacing discrete molecular structures with equivalent-continuum models. It has been shown that this replacement may be accomplished by equating the molecular potential energy of nano-structured materials with the mechanical strain energy of a representative continuum model. The development of an equivalent-truss model may be used as an intermediate step in establishing the equivalent-continuum model.

The proposed modeling method has been applied to determine the effective geometry and effective bending rigidity of a graphene sheet. A representative volume element (RVE) of the chemical structure of a graphene sheet has been substituted with RVEs of equivalent-truss and equivalent-continuum models. As a result, an effective thickness of the continuum model has been determined. This effective thickness has been shown to be significantly larger than the inter-planar spacing of graphite. The effective bending rigidity of an equivalent-continuum plate

model of a graphene sheet was also determined using the proposed method. The molecular potential energy of the molecular model of a graphene sheet subjected to cylindrical bending (to form a nanotube) was equated with the strain energy of an equivalent-continuum plate subjected to cylindrical bending.

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Table 1 - Ratio of calculated Young's modulus for different wall thicknesses with respect to the Young's modulus calculated with the inter-planar spacing

	Continuum wall thickness [nm]	Continuum cross-sectional area [nm ²]	Ratio of Young's moduli [%]
Load cases I and II	0.69	4.34r ^c	0.49
Load case III	0.57	3.58r ^c	0.60
Average of I, II, and III	0.65	4.08r ^c	0.52
Yakobson <i>et al.</i> 1996	0.07	0.44r ^c	4.86
Inter-planar spacing	0.34	2.14r ^c	1.00

Table 2 - Values of the force constant associated with bond inversion of a graphene sheet

Study	$\overline{K^0}$ [eV×nm ² /atom]
Bakowies and Thiel [36]	0.016
Robertson <i>et al.</i> - EP1 [43]	0.016
Robertson <i>et al.</i> - EP2 [43]	0.011
Robertson <i>et al.</i> - LDF [43]	0.021
Sawada and Hamada [44]	0.017
Miyamoto <i>et al.</i> [45]	0.020
Hernandez <i>et al.</i> (n,n) [46]	0.021
Hernandez <i>et al.</i> (n,0) [46]	0.022
Average	0.018

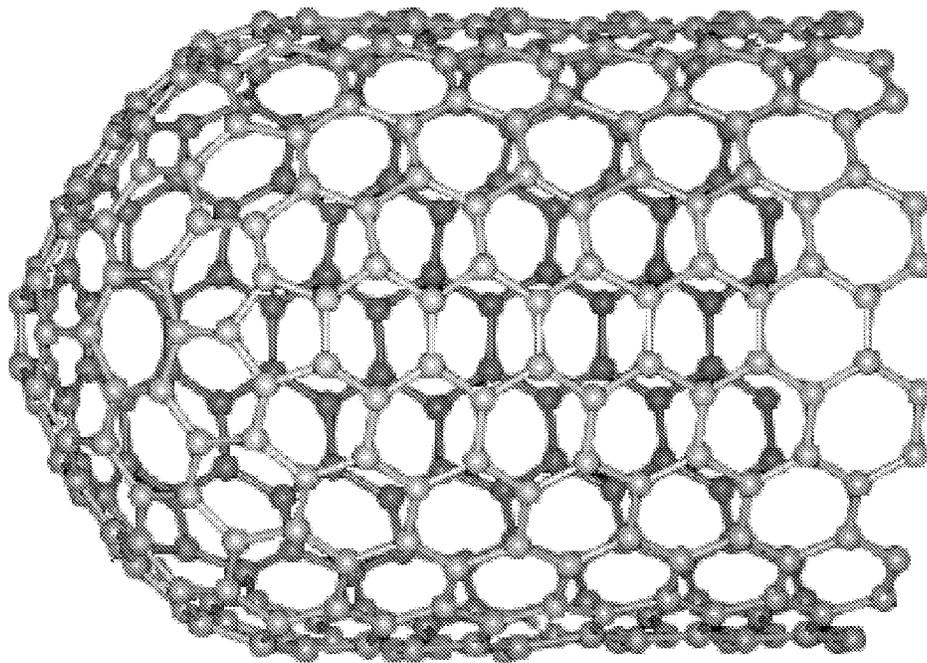


Figure 1 – End section of a single-walled carbon nanotube.

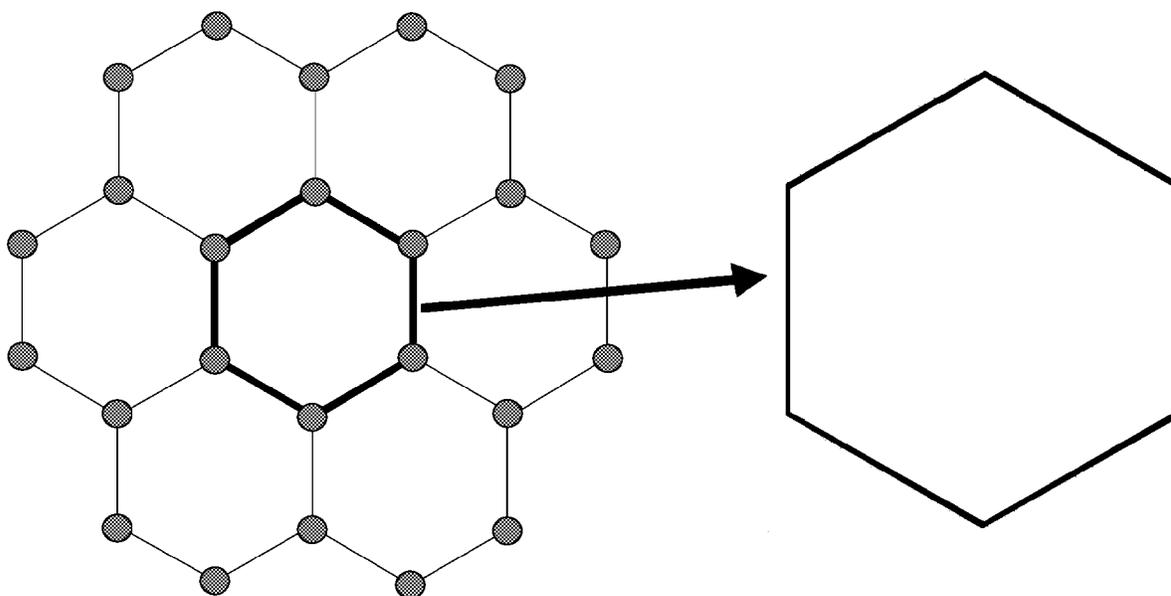


Figure 2 – Representative volume element of a graphene sheet.

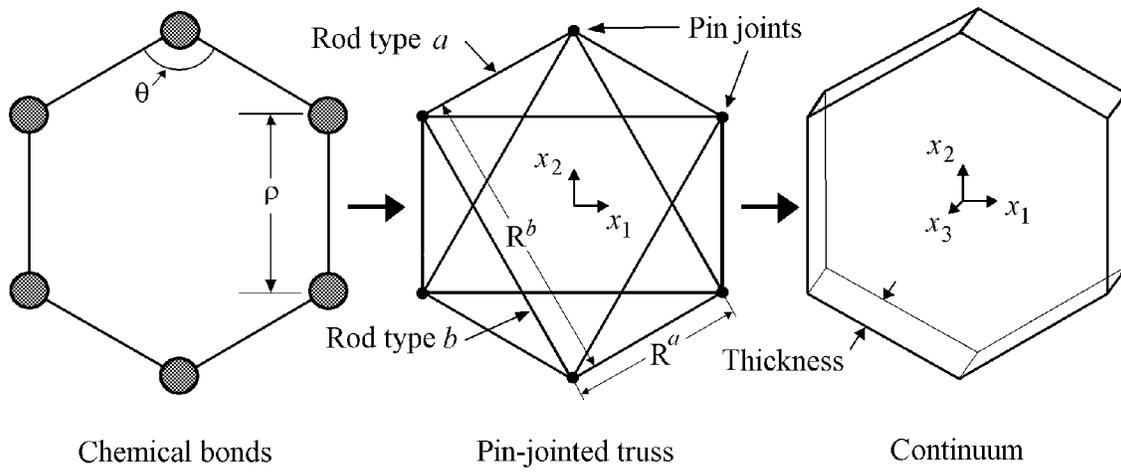


Figure 3 – Representative volume elements for the chemical, truss, and continuum models.

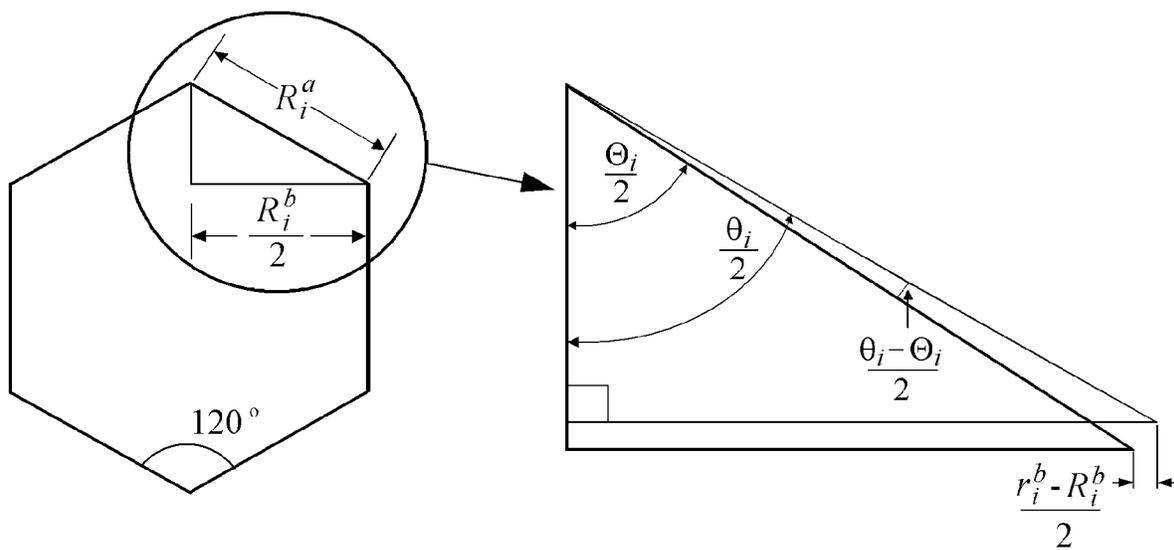


Figure 4 – Schematic of the deformed geometry of the representative volume element.

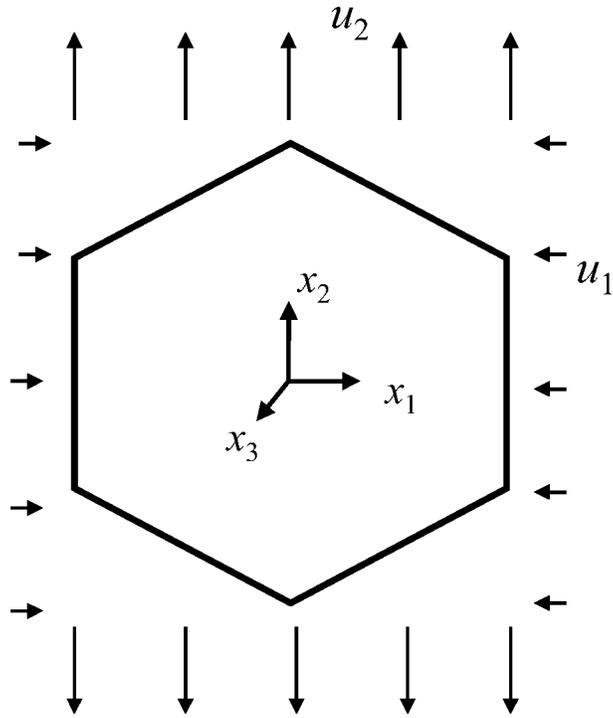


Figure 5 – Load case I: Extension along x_2 .

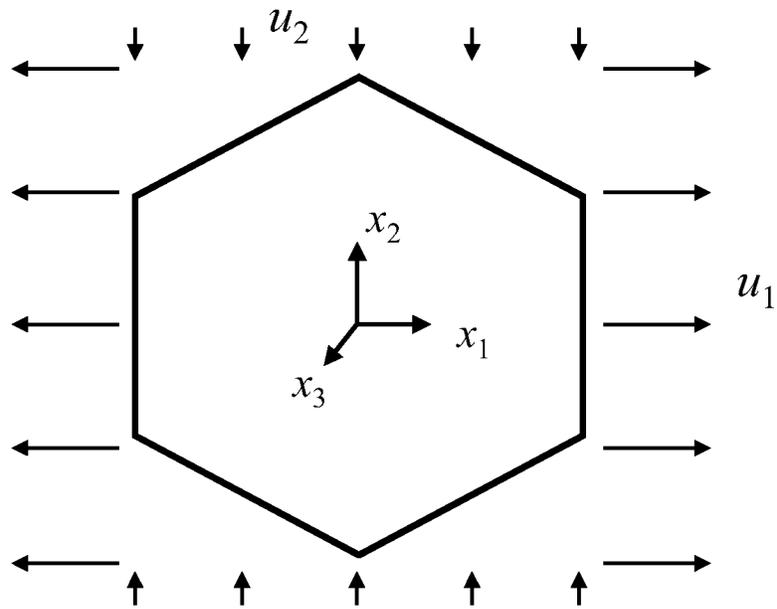


Figure 6 – Load case II: Extension along x_1 .

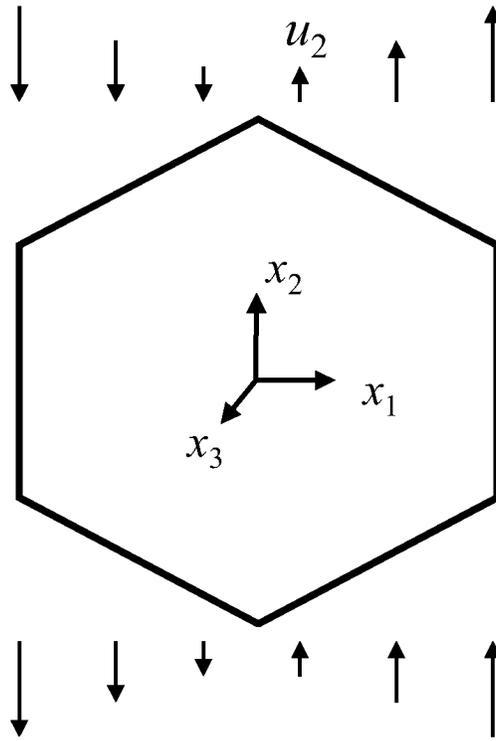


Figure 7 - Load case III: Pure shear.

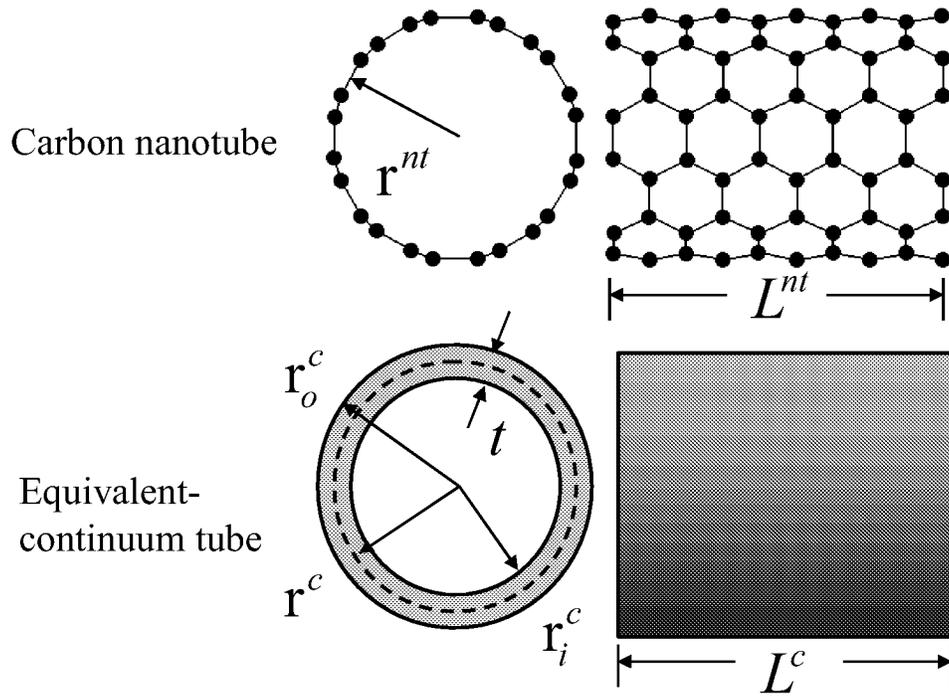


Figure 8 – Geometry of a carbon nanotube and an equivalent-continuum tube.

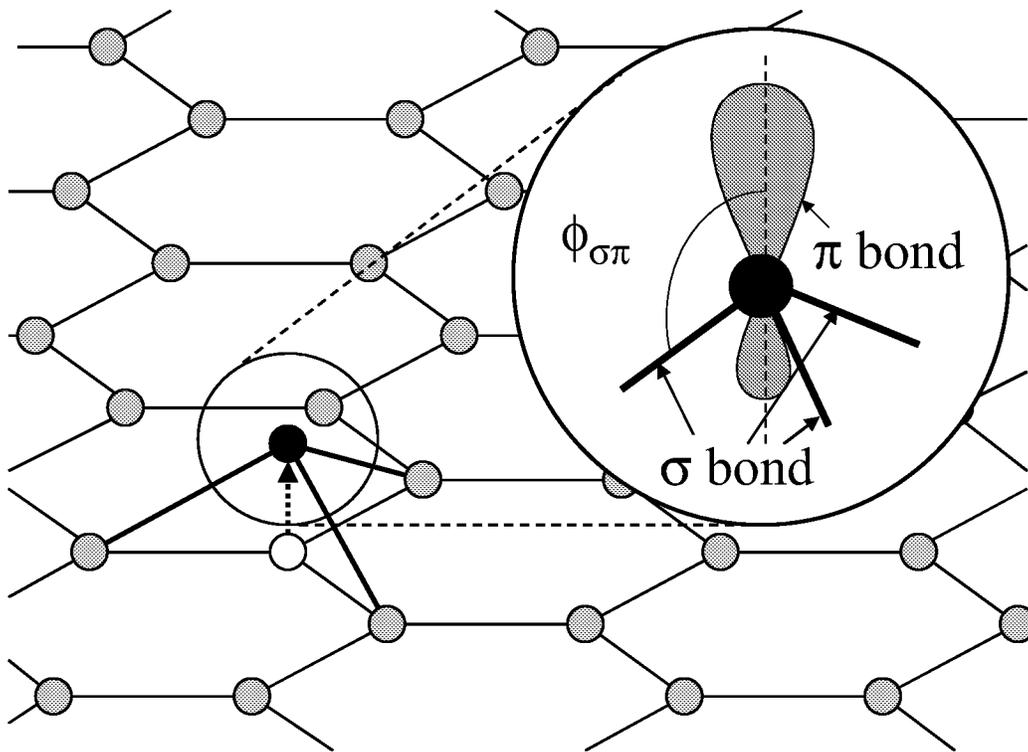


Figure 9 – Bond inversion of carbon atom in a graphene sheet.

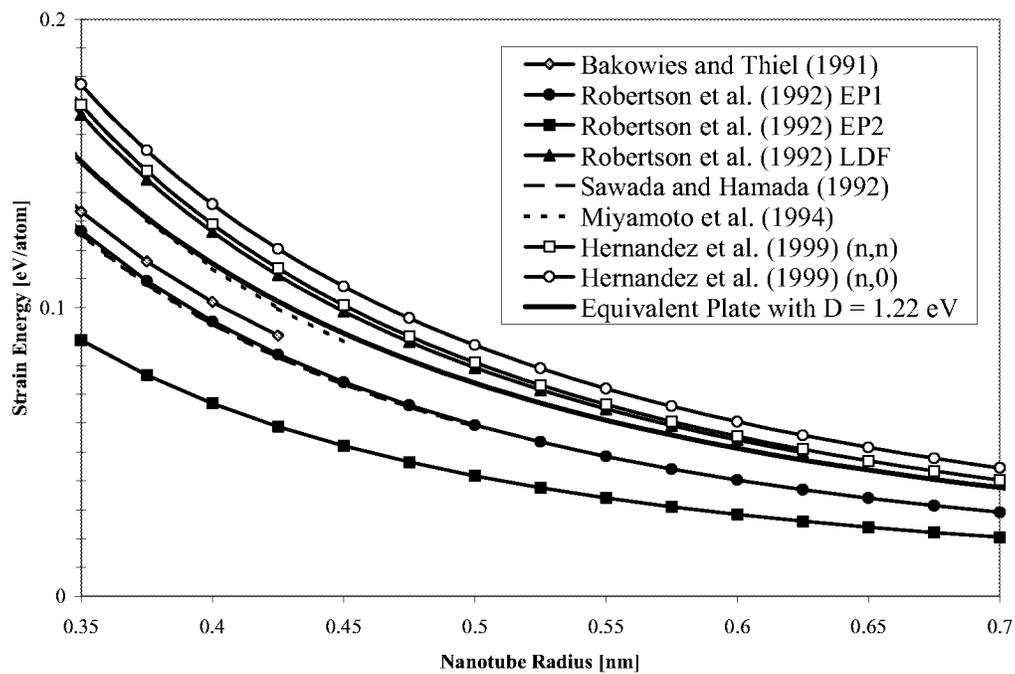


Figure 10 - Strain energy of a graphene sheet subjected to cylindrical bending.

REPORT DOCUMENTATION PAGE

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13. ABSTRACT (Maximum 200 words) A method has been proposed for developing structure-property relationships of nano-structured materials. This method serves as a link between computational chemistry and solid mechanics by substituting discrete molecular structures with equivalent-continuum models. It has been shown that this substitution may be accomplished by equating the vibrational potential energy of a nano-structured material with the strain energy of representative truss and continuum models. As important examples with direct application to the development and characterization of single-walled carbon nanotubes and the design of nanotube-based devices, the modeling technique has been applied to determine the effective-continuum geometry and bending rigidity of a graphene sheet. A representative volume element of the chemical structure of graphene has been substituted with equivalent-truss and equivalent-continuum models. As a result, an effective thickness of the continuum model has been determined. This effective thickness has been shown to be significantly larger than the interatomic spacing of graphite. The effective thickness has been shown to be significantly larger than the inter-planar spacing of graphite. The effective bending rigidity of the equivalent-continuum model of a graphene sheet was determined by equating the vibrational potential energy of the molecular model of a graphene sheet subjected to cylindrical bending with the strain energy of an equivalent-continuum plate subjected to cylindrical bending.			
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